

Multivariate Normal Distribution II

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Detour: Inverse of partioned symmetric matrix ¹

Consider an $n \times n$ symmetric matrix A and divide it into four blocks

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} \\ A_{12}^T & A_{22} \end{bmatrix}$$

For example, let $n = 3$, we have

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 5 & 6 \\ 3 & 6 & 8 \end{bmatrix}$$

We could for example have

$$A_{11} = \begin{bmatrix} 1 & 2 \\ 2 & 5 \end{bmatrix} \text{ and } A_{12} = \begin{bmatrix} 3 \\ 6 \end{bmatrix} \text{ and } A_{22} = [8]$$

¹Courtesy: <http://fourier.eng.hmc.edu/e161/lectures/gaussianprocess/node6.html>

Detour: Inverse of partitioned symmetric matrix

Question: Write $B = A^{-1}$ in terms of the four blocks

$$B = \begin{bmatrix} B_{11} & B_{12} \\ B_{12}^T & A_{22} \end{bmatrix} = A^{-1}$$

$$A_{11} \text{ and } B_{11} \in R^{p \times p}$$

$$A_{22} \text{ and } B_{22} \in R^{q \times q}$$

$$A_{12} = A_{21}^T \text{ and } B_{12} = B_{21}^T \in R^{p \times q}$$

$$\text{and, } p + q = n$$

Detour: Inverse of partitioned symmetric matrix

$$\begin{aligned} I_n &= AA^{-1} = AB \\ &= \begin{bmatrix} A_{11} & A_{12} \\ A_{12}^T & A_{22} \end{bmatrix} \begin{bmatrix} B_{11} & B_{12} \\ B_{12}^T & B_{22} \end{bmatrix} = \\ &\begin{bmatrix} A_{11}B_{11} + A_{12}B_{12}^T & A_{11}B_{12} + A_{12}A_{22} \\ A_{12}^TB_{11} + A_{22}B_{12}^T & A_{12}^TB_{12} + A_{22}B_{22} \end{bmatrix} = \begin{bmatrix} I_p & 0 \\ 0 & I_q \end{bmatrix} \end{aligned}$$

Thus, we have

$$\begin{aligned} A_{11}B_{11} + A_{12}B_{12}^T &= I_p \\ A_{11}B_{12} + A_{12}A_{22} &= 0^{p \times q} \\ A_{12}^TB_{11} + A_{22}B_{12}^T &= 0^{q \times p} \\ A_{12}^TB_{12} + A_{22}B_{22} &= I_q \end{aligned}$$

Detour: Inverse of partitioned symmetric matrix

Moving the expressions around we get the following results.

$$B_{11} = (A_{11} - A_{12}A_{22}^{-1}A_{12}^T)^{-1} = A_{11}^{-1} + A_{11}^{-1}A_{12}(A_{22} - A_{12}^T A_{11}^{-1}A_{12})^{-1}A_{12}^T$$

$$B_{22} = (A_{22} - A_{12}^T A_{11}^{-1}A_{12})^{-1} = A_{22}^{-1} + A_{22}^{-1}A_{12}^T(A_{11} - A_{12}A_{22}^{-1}A_{12}^T)^{-1}A_{12}$$

$$B_{12}^T = -A_{22}^{-1}A_{12}^T(A_{11} - A_{12}A_{22}^{-1}A_{12}^T)^{-1}$$

$$B_{12}^T = -A_{11}^{-1}A_{12}^T(A_{22} - A_{12}^T A_{11}^{-1}A_{12})^{-1}$$

Determinant of Partitioned Symmetric Matrix

Theorem: Determinant of a partitioned symmetric matrix can be written as follows

$$\begin{aligned} |A| &= \left| \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \right| \\ &= |A_{11}| |A_{22} - A_{12}^T A_{11}^{-1} A_{12}| \\ &= |A_{22}| |A_{11} - A_{12} A_{22}^{-1} A_{12}^T| \end{aligned}$$

Determinant of Partitioned Symmetric Matrix

Proof: Note that

$$\begin{aligned} A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} &= \begin{bmatrix} A_{11} & 0 \\ A_{12}^T & I \end{bmatrix} \begin{bmatrix} I & A_{11}^{-1}A_{12} \\ 0 & A_{22} - A_{12}^T A_{11}^{-1} A_{12} \end{bmatrix} \\ &= \begin{bmatrix} I & A_{12} \\ 0 & A_{22} \end{bmatrix} \begin{bmatrix} A_{11} - A_{12}A_{22}^{-1}A_{12}^T & 0 \\ A_{22}^{-1}A_{21} & I \end{bmatrix} \end{aligned}$$

The theorem is proved as we also know that

$$|AB| = |A||B|$$

and

$$\begin{vmatrix} B & 0 \\ C & D \end{vmatrix} = \begin{vmatrix} B & C \\ 0 & D \end{vmatrix} = |B| |D|$$

Marginalisation and Conditional of multivariate normal²

Assume an n -dimensional random vector

$$\mathbf{x} = \begin{bmatrix} \mathbf{x}_1 & \mathbf{x}_2 \end{bmatrix}$$

has a normal distribution $N(\mathbf{x}, \mu, \Sigma)$ with

$$\mu = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix} \text{ and } \Sigma = \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix}$$

where \mathbf{x}_1 and \mathbf{x}_2 are two subvectors of respective dimensions p and q with $p + q = n$. Note that $\Sigma = \Sigma^T$, and $\Sigma_{21} = \Sigma_{12}^T$.

²Courtesy: <http://fourier.eng.hmc.edu/e161/lectures/gaussianprocess/node7.html>.

Marginalisation and Conditional of multivariate normal

Theorem:

part a: The marginal distributions of \mathbf{x}_1 and \mathbf{x}_2 are also normal with mean vector μ_i and covariance matrix Σ_{ii} ($i = 1, 2$), respectively.

part b: The conditional distribution of \mathbf{x}_i given \mathbf{x}_j is also normal with mean vector

Marginalisation and Conditional of multivariate normal

Proof:

The joint density of \mathbf{x} is:

$$f(\mathbf{x}) = f(\mathbf{x}_1, \mathbf{x}_2) = \frac{1}{(2\pi)^{n/2} |\Sigma|^{1/2}} \exp\left[-\frac{1}{2} Q(\mathbf{x}_1, \mathbf{x}_2)\right]$$

where Q is defined as

$$\begin{aligned} Q(\mathbf{x}_1, \mathbf{x}_2) &= (\mathbf{x} - \boldsymbol{\mu})^T \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu}) \\ &= [(\mathbf{x}_1 - \boldsymbol{\mu}_1)^T, (\mathbf{x}_2 - \boldsymbol{\mu}_2)^T] \begin{bmatrix} \Sigma^{11} & \Sigma^{12} \\ \Sigma^{21} & \Sigma^{22} \end{bmatrix} \begin{bmatrix} \mathbf{x}_1 - \boldsymbol{\mu}_1 \\ \mathbf{x}_2 - \boldsymbol{\mu}_2 \end{bmatrix} \\ &= (\mathbf{x}_1 - \boldsymbol{\mu}_1)^T \Sigma^{11} (\mathbf{x}_1 - \boldsymbol{\mu}_1) + 2(\mathbf{x}_1 - \boldsymbol{\mu}_1)^T \Sigma^{12} (\mathbf{x}_2 - \boldsymbol{\mu}_2) + (\mathbf{x}_2 - \boldsymbol{\mu}_2)^T \dots \\ &\quad \dots \Sigma^{22} (\mathbf{x}_2 - \boldsymbol{\mu}_2) \end{aligned}$$

Marginalisation and Conditional of multivariate normal

Here we have assumed

$$\Sigma^{-1} = \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix}^{-1} = \begin{bmatrix} \Sigma^{11} & \Sigma^{12} \\ \Sigma^{21} & \Sigma^{22} \end{bmatrix}$$

According to inverse of a partitioned symmetric matrix we have,

$$\Sigma^{11} = \left(\Sigma_{11} - \Sigma_{12} \Sigma_{22}^{-1} \Sigma_{12}^T \right)^{-1} = \Sigma_{11}^{-1} + \Sigma_{11}^{-1} \Sigma_{12} \left(\Sigma_{22} - \Sigma_{12}^T \Sigma_{11}^{-1} \Sigma_{12} \right)^{-1}$$

$$\Sigma^{22} = \left(\Sigma_{22} - \Sigma_{12}^T \Sigma_{11}^{-1} \Sigma_{12} \right)^{-1} = \Sigma_{22}^{-1} + \Sigma_{22}^{-1} \Sigma_{12}^T \left(\Sigma_{11} - \Sigma_{12} \Sigma_{22}^{-1} \Sigma_{12}^T \right)^{-1}$$

$$\Sigma^{12} = -\Sigma_{11}^{-1} \Sigma_{12} \left(\Sigma_{22} - \Sigma_{12}^T \Sigma_{11}^{-1} \Sigma_{12} \right)^{-1} = (\Sigma^{21})^T$$

Marginalisation and Conditional of multivariate normal

Substituting the second expression for Σ^{11} , first expression for Σ^{22} , and Σ^{12} into $Q(\mathbf{x}_1, \mathbf{x}_2)$ to get:

$$\begin{aligned}
 Q(\mathbf{x}_1, \mathbf{x}_2) &= (\mathbf{x}_1 - \mu_1)^T \left[\Sigma_{11}^{-1} + \Sigma_{11}^{-1} \Sigma_{12} \left(\Sigma_{22} - \mathbf{A}_{12}^T \Sigma_{11}^{-1} \Sigma_{12} \right)^{-1} \Sigma_{12}^T \Sigma_{11}^{-1} \right. \\
 &\quad \left. - 2 (\mathbf{x}_1 - \mu_1)^T \left[\Sigma_{11}^{-1} \Sigma_{12} \left(\Sigma_{22} - \Sigma_{12}^T \Sigma_{11}^{-1} \Sigma_{12} \right)^{-1} \right] (\mathbf{x}_2 - \mu_2) \right. \\
 &\quad \left. + (\mathbf{x}_2 - \mu_2)^T \left[\left(\Sigma_{22} - \Sigma_{12}^T \Sigma_{11}^{-1} \Sigma_{12} \right)^{-1} \right] (\mathbf{x}_2 - \mu_2) \right] \\
 &= (\mathbf{x}_1 - \mu_1)^T \Sigma_{11}^{-1} (\mathbf{x}_1 - \mu_1) \\
 &\quad + (\mathbf{x}_1 - \mu_1)^T \Sigma_{11}^{-1} \Sigma_{12} \left(\Sigma_{22} - \mathbf{A}_{12}^T \Sigma_{11}^{-1} \Sigma_{12} \right)^{-1} \Sigma_{12}^T \Sigma_{11}^{-1} (\mathbf{x}_1 - \mu_1) \\
 &\quad - 2 (\mathbf{x}_1 - \mu_1)^T \left[\Sigma_{11}^{-1} \Sigma_{12} \left(\Sigma_{22} - \Sigma_{12}^T \Sigma_{11}^{-1} \Sigma_{12} \right)^{-1} \right] (\mathbf{x}_2 - \mu_2) \\
 &\quad + (\mathbf{x}_2 - \mu_2)^T \left[\left(\Sigma_{22} - \Sigma_{12}^T \Sigma_{11}^{-1} \Sigma_{12} \right)^{-1} \right] (\mathbf{x}_2 - \mu_2)
 \end{aligned}$$

Marginalisation and Conditional of multivariate normal

$$\begin{aligned} &= (\mathbf{x}_1 - \mu_1)^T \Sigma_{11}^{-1} \\ &\quad + \left[(\mathbf{x}_2 - \mu_2) - \Sigma_{12}^T \Sigma_{11}^{-1} (\mathbf{x}_1 - \mu_1) \right]^T \left(\Sigma_{22} - \Sigma_{12}^T \Sigma_{11}^{-1} \Sigma_{12} \right)^{-1} \left[(\mathbf{x}_2 - \mu_2) - \Sigma_{12}^T \Sigma_{11}^{-1} (\mathbf{x}_1 - \mu_1) \right] \end{aligned}$$

The last equal sign is due to the following equations for any vectors u and v and a symmetric matrix $A = A^T$:

$$\begin{aligned} &u^T A u - 2u^T A v + v^T A v = u^T A u - u^T A v - u^T A v + v^T A v \\ &= u^T A (u - v) - (u - v)^T A v = u^T A (u - v) - v^T A (u - v) \\ &= (u - v)^T A (u - v) = (v - u)^T A (v - u) \end{aligned}$$

Marginalisation and Conditional of multivariate normal

We define $b \triangleq \mu_2 + \Sigma_{12}^T \Sigma_{11}^{-1} (\mathbf{x}_1 - \mu_1)$

$$A \triangleq \Sigma_{22} - \Sigma_{12}^T \Sigma_{11}^{-1} \Sigma_{12}$$

and

$$\begin{cases} Q_1(x_1) \triangleq (x_1 - \mu_1)^T \Sigma_1^{-1} (x_1 - \mu_1) \\ Q_2(x_1, x_2) \triangleq [(x_2 - \mu_2) - \Sigma_{12}^T \Sigma_{11}^{-1} (x_1 - \mu_1)]^T (\Sigma_{22} - \Sigma_{12}^T \Sigma_{11}^{-1} \Sigma_{12})^{-1} \\ \quad \times [(x_2 - \mu_2) - \Sigma_{12}^T \Sigma_{11}^{-1} (x_1 - \mu_1)] \\ = (x_2 - b)^T A^{-1} (x_2 - b) \end{cases}$$

and get

$$Q(\mathbf{x}_1, \mathbf{x}_2) = Q_1(\mathbf{x}_1) + Q_2(\mathbf{x}_1, \mathbf{x}_2)$$

Marginalisation and Conditional of multivariate normal

Now the joint distribution can be written as:

$$\begin{aligned} f(\mathbf{x}) &= f(\mathbf{x}_1, \mathbf{x}_2) = \frac{1}{(2\pi)^{n/2} |\Sigma|^{1/2}} \exp \left[-\frac{1}{2} \mathbf{Q}(\mathbf{x}_1, \mathbf{x}_2) \right] \\ &= \frac{1}{(2\pi)^{n/2} |\Sigma_{11}|^{1/2} |\Sigma_{22} - \Sigma_{12}^T \Sigma_{11}^{-1} \Sigma_{12}|^{1/2}} \exp \left[-\frac{1}{2} \mathbf{Q}(\mathbf{x}_1, \mathbf{x}_2) \right] \\ &= \frac{1}{(2\pi)^{p/2} |\Sigma_{11}|^{1/2}} \exp \left[-\frac{1}{2} (\mathbf{x}_1 - \mu_1)^T \Sigma_{11}^{-1} (\mathbf{x}_1 - \mu_1) \right] \frac{1}{(2\pi)^{q/2} |\mathbf{A}|^{1/2}} \\ &= N(\mathbf{x}_1, \mu_1, \Sigma_{11}) N(\mathbf{x}_2, \mathbf{b}, \mathbf{A}) \end{aligned}$$

The third equal sign is due to Determinant of a partitioned symmetric matrix:

$$|\Sigma| = |\Sigma_{11}| |\Sigma_{22} - \Sigma_{12}^T \Sigma_{11}^{-1} \Sigma_{12}|$$

Marginalisation and Conditional of multivariate normal

The marginal distribution of \mathbf{x}_1 is

$$f_1(\mathbf{x}_1) = \int f(\mathbf{x}_1, \mathbf{x}_2) d\mathbf{x}_2 = \frac{1}{(2\pi)^{p/2} |\Sigma_{11}|^{1/2}} \exp \left[-\frac{1}{2} (\mathbf{x}_1 - \mu_1)^T \Sigma_{11}^{-1} (\mathbf{x}_1 - \mu_1) \right]$$

and the conditional distribution of \mathbf{x}_2 given \mathbf{x}_1 is

$$f_{2|1}(\mathbf{x}_2|\mathbf{x}_1) = \frac{f(\mathbf{x}_1, \mathbf{x}_2)}{f(\mathbf{x}_1)} = \frac{1}{(2\pi)^{q/2} |\mathbf{A}|^{1/2}} \exp \left[-\frac{1}{2} (\mathbf{x}_2 - \mathbf{b})^T \mathbf{A}^{-1} (\mathbf{x}_2 - \mathbf{b}) \right]$$

Marginalisation and Conditional of multivariate normal

with

$$\mathbf{b} = \mu_2 + \Sigma_{12}^T \Sigma_{11}^{-1} (\mathbf{x}_1 - \mu_1)$$

$$\mathbf{A} = \Sigma_{22} - \Sigma_{12}^T \Sigma_{11}^{-1} \Sigma_{12}$$